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Possible f -wave superconductivity in Sr_2RuO_4 ?

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Abstract. – Until recently it has been believed that the superconductivity in Sr_2RuO_4 is described by p -wave pairing. However, both the recent specific heat and the magnetic penetration depth measurements on the purest single crystals of Sr_2RuO_4 appear to be explained more consistently in terms of f -wave superconductivity. In order to further this hypothesis, we study theoretically the thermodynamics and thermal conductivity of f -wave superconductors in a planar magnetic field. We find the simple expressions for these quantities when $H \ll H_{c2}$ and $T \ll T_c$, which should be readily accessible experimentally.

Introduction. – The recently discovered superconductivity in Sr_2RuO_4 has been believed to be described in terms of p -wave superconductor with the full energy gap [1, 2]. For example, the spontaneous spin polarization seen by muon spin rotation experiment [3] and the flat Knight shift seen by NMR [4], are consistent with the triplet pairing. However, the recent specific heat, T_1^{-1} in NMR [5] and the superfluid density of the purest Sr_2RuO_4 single crystals with $T_c = 1.5$ K [6] are inconsistent with the p -wave superconductivity.

The T^2 -dependence of the specific heat, the T^3 -dependence of T_1^{-1} , and the T -dependence of the superfluid density indicate clearly the presence of the nodal structure in the superconducting order parameter. One possible interpretation is that the superconducting order parameter in the γ -band has the full gap as assumed earlier, while the ones in the α - and β -band have the nodal structure [7].

Alternatively, we may consider the possibility that the superconducting order parameters in these 3 bands are the same and described by f -wave superconductor with the order parameter [8]

$$\mathbf{d}(\mathbf{k}) = \frac{3\sqrt{3}}{2} \Delta \hat{d} \hat{k}_3 (\hat{k}_1 \pm i \hat{k}_2)^2 \quad (1)$$

with $\hat{d} \parallel \hat{c}$ which is believed to describe the superconductivity in UPt_3 [9]. Indeed the overall temperature dependence of the specific heat [5] and the superfluid density [6] are described

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Fig. 1. – The specific heat data [5] divided by γT where γ is Sommerfeld constant is compared with the theoretical results for the isotropic p -wave [7] and f -wave [8] superconductors.

Fig. 2. – The superfluid density data of single crystal Sr_2RuO_4 [6] is compared with the theoretical results of p -wave [7] and f -wave [8] superconductors.

much more consistently by f -wave superconductor. We compare the experimental data of the specific heat [5] and the superfluid density [6] of Sr_2RuO_4 crystals with the theoretical results for the weak coupling p -wave and f -wave superconductors in Fig.1 and Fig.2, respectively. Of course, there are still obvious discrepancies in this identification. For example, the data for $C_s(T)/\gamma T$ exhibits weakly convex behavior while the theory predicts weakly concave behavior, though the discrepancy is not so striking. Also the theory cannot account for the T^3 -dependence of the superfluid density observed in the less pure samples. But this may be due to the non-locality effect suggested by Kosztin and Leggett [10].

In a recent series of papers [11, 12], we have proposed that the thermal conductivity tensor in a planar magnetic field near H_{c2} provide the crucial test of the symmetry of the underlying superconductivity. We recall also ingenious thermal conductivity experiments [13, 14] have been carried out to elucidate the nodal structure of d -wave superconductivity in YBCO.

In the following we take the superconducting order parameter given by Eq.(1), and first study the quasi-particle density of states in the presence of both magnetic field and impurities. Starting from the pioneering work by Volovik [15], we have fully developed technology for this purpose, at least, for $H \ll H_{c2}$ and $T \ll T_c$ [16, 17, 18, 19]. The central idea is to introduce the effect of the magnetic field or the supercurrent in the quasi-particle spectrum through the Doppler shift[20]. When computing the effect of the magnetic field to the quasi-particle density of states, for example, we take the average of terms containing the Doppler shift over both the quasi-particle momentum and over the Wigner-Seitz cell containing a single vortex in a real space. Further impurity scattering is treated in the unitarity limit as in most of unconventional superconductors [8].

Perhaps the most important result is that the thermal conductivity tensors exhibit significant $\tilde{\theta}$ -dependence, where $\tilde{\theta}$ is the angle between the magnetic field and the heat current both lying in the a - b plane. Recently the thermal conductivity of Sr_2RuO_4 in a planar magnetic field has been measured, which does not exhibit clear $\tilde{\theta}$ -dependence [21, 22]. Of course the $\tilde{\theta}$ -dependence we found for f -wave superconductor is much smaller than the one found for p -wave superconductor [23], but should be still visible. Therefore it appears that the thermal conductivity data exclude both p - and f -wave superconductors from the candidate for superconductivity in Sr_2RuO_4 . Clearly we have to look for another candidate.

On the other hand, the present result should apply to UPt_3 in a low magnetic field with a heat current within the a - b plane. We have already studied the thermal conductivity of f -wave superconductor in the vicinity of H_{c2} [12]. Indeed this calculation reproduces the $\tilde{\theta}$ -dependence of the thermal conductivity of UPt_3 observed by Suderow et al [24].

Quasi-particle density of states, the specific heat, and superfluid density. – In the following we shall use the approach given in [16]. The residual density of states in f -wave superconductors is given by

$$\frac{N(\omega=0)}{N_0} = \text{Re} \left\langle \frac{\tilde{\omega} - \mathbf{v} \cdot \mathbf{q}}{\sqrt{(\tilde{\omega} - \mathbf{v} \cdot \mathbf{q})^2 - \Delta^2 |f|^2}} \right\rangle \Big|_{\omega=0}$$

$$\simeq \frac{1}{\sqrt{3}} \langle \ln \left(\frac{2}{\sqrt{C_0^2 + x^2}} \right) + x \tan^{-1} \left(\frac{x}{C_0} \right) \rangle \quad (2)$$

where $f = \frac{3\sqrt{3}}{2} \cos \theta (1 - \cos^2 \theta)$, $x = |\mathbf{v} \cdot \mathbf{q}|/\Delta$ with \mathbf{v} the Fermi velocity, \mathbf{q} the superfluid momentum, and $C_0 = -i \frac{\tilde{\omega}}{\Delta} \big|_{\omega=0}$ with $\tilde{\omega}$ the renormalized frequency [19]. In deriving Eq.(2), we have assumed C_0 , $x \ll 1$. Now in the unitarity limit of the impurity scattering we obtain [8]

$$C_0 = \frac{\Gamma}{\Delta} / \left(\frac{N(\omega=0)}{N_0} \right) \quad (3)$$

and Γ and Δ are the impurity scattering rate and the superconducting order parameter, respectively.

We can solve Eq.(2) and (3) analytically in the two limiting cases:

a) superclean limit ($C_0 \ll \langle x \rangle \ll 1$, i.e. $\frac{\Gamma}{\Delta} \ll \frac{H}{H_{c2}} \ll 1$)

$$\frac{N(H)}{N_0} \simeq \frac{\pi}{2\sqrt{3}} \langle x \rangle + \frac{2}{\pi} \frac{\Gamma}{\Delta \langle x \rangle} \langle \ln \left(\frac{2}{x} \right) - 1 \rangle \quad (4)$$

and

$$C_0 \simeq \frac{2\sqrt{3}}{\pi} \frac{\Gamma}{\Delta \langle x \rangle} \quad (5)$$

Finally, following [17] the spatial average gives

$$\frac{N(H)}{N_0} \simeq \frac{1}{\sqrt{3}} \frac{\sqrt{vv'eH}}{\Delta} + \frac{\Gamma}{\sqrt{vv'eH}} \ln \left(\frac{4\Delta}{\sqrt{vv'eH}} \right) \quad (6)$$

where $\langle x \rangle \simeq \frac{2}{\pi} \frac{\sqrt{vv'eH}}{\Delta}$ and $\langle \ln x \rangle \simeq \ln \left(\frac{\sqrt{vv'eH}}{2\Delta} \right)$ after the spatial average. Here v and v' are the Fermi velocity in the a - b plane and parallel to the c -axis, respectively. As shown by Volovik [15] already the density of states increases like \sqrt{H} for $H \ll H_{c2}$.

b) clean limit ($\langle x \rangle \ll C_0 \ll 1$, i.e. $\frac{H}{H_{c2}} \ll \frac{\Gamma}{\Delta} \ll 1$)

$$\begin{aligned} \frac{N(H)}{N_0} &\simeq \frac{N_{\text{imp}}}{N_0} \left(1 + \frac{\Delta}{2\sqrt{3}\Gamma} \langle x^2 \rangle \right) \\ &= \frac{N_{\text{imp}}}{N_0} \left(1 + \frac{vv'eH}{8\sqrt{3}\Gamma\Delta} \ln \left(\frac{2\Delta}{\sqrt{vv'eH}} \right) \right) \end{aligned} \quad (7)$$

and

$$C_0^2 \ln \left(\frac{2}{C_0} \right) \simeq \sqrt{3} \frac{\Gamma}{\Delta} - \frac{1}{2} \langle x^2 \rangle \quad (8)$$

where

$$\frac{N_{\text{imp}}}{N_0} \simeq \sqrt{\frac{\Gamma}{2\sqrt{3}\Delta} \ln \left(\frac{4\Delta}{\sqrt{3}\Gamma} \right)} \quad (9)$$

Here $\frac{N_{\text{imp}}}{N_0}$ is the density of states in the $H = 0$ case with the unitarity impurity scatterer.

Also, unlike in d -wave superconductors [18, 19], the specific heat is independent of the direction of the planar magnetic field. Making use of N/N_0 given in Eqs. (5) and (8) the low temperature specific heat and the superfluid density are expressed as in [25]

$$C_s(T, H) = \frac{2\pi^2}{3} T N(H) \quad (10)$$

and

$$\rho_s(H, T = 0) = 1 - N(H)/N_0 \quad (11)$$

Thermal conductivity tensor. – As already discussed, the angular independence of the thermal conductivity tensor in a planar magnetic field appears to offer the test of f -wave superconductivity. Following the formalism developed by Ambegaokar-Griffin [26], the thermal conductivity tensor for $T \ll \Delta_0$ is given by

$$\kappa_{\parallel}/\kappa_n = 3 \frac{\Gamma}{\Delta} \left\langle (1 - \cos^2 \theta) \cos^2 \phi \frac{\frac{1}{2} \left(1 + \frac{C_0^2 + x^2 - |f|^2}{|(C_0 + ix)^2 + |f|^2|} \right)}{\text{Re} \sqrt{(C_0 + ix)^2 + |f|^2}} \right\rangle \quad (12)$$

and

$$\kappa_{\perp}/\kappa_n = \frac{3}{2} \frac{\Gamma}{\Delta} \left\langle (1 - \cos^2 \theta) \sin(2\phi) \frac{\frac{1}{2} \left(1 + \frac{C_0^2 + x^2 - |f|^2}{|(C_0 + ix)^2 + |f|^2|} \right)}{\text{Re} \sqrt{(C_0 + ix)^2 + |f|^2}} \right\rangle \quad (13)$$

and $\kappa_n = \frac{\pi^2 T n}{6 \Gamma m}$, the thermal conductivity in the normal state.

a) superclean limit ($C_0 \ll \langle x \rangle \ll 1$, i.e. $\frac{H}{H_{c2}} \ll \frac{\Gamma}{\Delta} \ll 1$)

Making use of C_0 obtained in Eq.(5) and integrating over $\cos \theta$ and ϕ , we obtain

$$\kappa_{\parallel}/\kappa_n \simeq \frac{1}{6} \frac{v v' e H}{\Delta^2} (1 - \frac{1}{3} \cos(2\tilde{\theta})) \quad (14)$$

and

$$\kappa_{\perp}/\kappa_n \simeq -\frac{1}{18} \frac{v v' e H}{\Delta^2} \sin(2\tilde{\theta}) \quad (15)$$

where $\tilde{\theta}$ is the angle between \mathbf{H} and \mathbf{q} the heat current within the a - b plane. The above expressions may be contrasted with those in d -wave superconductors which is given by [19]

$$\kappa_{\parallel}/\kappa_n \simeq \frac{2}{\pi} \frac{v v' e H}{\Delta^2} (0.955 + 0.0286 \cos(4\tilde{\theta}))^2 \quad (16)$$

and

$$\kappa_{\perp}/\kappa_n \simeq -\frac{2}{\pi} \frac{v v' e H}{\Delta^2} (0.955 + 0.0286 \cos(4\tilde{\theta})) (0.29 \sin(2\tilde{\theta})) \quad (17)$$

For $\frac{T}{\Delta} \gg C_0$, κ_{\parallel} is given by

$$\kappa_{\parallel}(H = 0) = \frac{3\sqrt{3}\zeta(3)T^2}{2\Delta\sqrt{\sqrt{3}\Gamma\Delta}} \sqrt{\ln(2\sqrt{\frac{\Delta}{\sqrt{3}\Gamma}}) \frac{n}{m}} \quad (18)$$

and $\zeta(3) = 1.202\dots$. In this limit the thermal conductivity increase like T^2 as in d -wave superconductors [19].

b) clean limit ($\langle x \rangle \ll C_0 \ll 1$, i.e. $\frac{\Gamma}{\Delta} \ll \frac{H}{H_{c2}} \ll 1$)

$$\begin{aligned} \kappa_{\parallel}/\kappa_0 &\simeq 1 + \frac{1}{3} \frac{\langle (1 + \cos(2\phi))x^2 \rangle}{C_0^2} \\ &= 1 + \frac{1}{12\sqrt{3}} \left(1 - \frac{1}{2} \cos(2\tilde{\theta})\right) \frac{vv'eH}{\Gamma\Delta} \ln\left(2\sqrt{\frac{\Delta}{\sqrt{3}\Gamma}}\right) \ln\left(\frac{2\Delta}{\sqrt{vv'eH}}\right) \end{aligned} \quad (19)$$

$$\kappa_{\perp}/\kappa_0 \simeq -\frac{1}{24\sqrt{3}} \sin(2\tilde{\theta}) \frac{vv'eH}{\Gamma\Delta} \ln\left(2\sqrt{\frac{\Delta}{\sqrt{3}\Gamma}}\right) \ln\left(\frac{2\Delta}{\sqrt{vv'eH}}\right) \quad (20)$$

where $\kappa_0 = \frac{\pi^2 T n}{6\sqrt{3}\Delta m}$ is Lee's universal thermal conductivity [27]. Therefore $\kappa_{\perp} \sim -\sin(2\tilde{\theta})$ appears to be the universal behavior for p -wave, d -wave, and f -wave superconductors.

For $\mathbf{H} \parallel \mathbf{c}$, we can derive the corresponding expressions readily, though we don't expect any angular dependence. The quasi-particle density of states is given by for the superclean limit,

$$N(H)/N_0 \simeq \frac{\pi}{2\sqrt{3}} \frac{v\sqrt{eH}}{\Delta^2} + \frac{2}{\pi} \frac{\Gamma}{v\sqrt{eH}} \ln\left(\frac{4\Delta}{v\sqrt{eH}}\right) \quad (21)$$

for the superclean limit, and

$$N(H)/N_0 \simeq \frac{N_{\text{imp}}}{N_0} \left(1 + \frac{v^2 eH}{4\sqrt{3}\Gamma\Delta} \ln\left(\frac{2\Delta}{v\sqrt{eH}}\right)\right) \quad (22)$$

for the clean limit. Also the thermal conductivity tensor is given by

$$\kappa_{\parallel}/\kappa_n \simeq \frac{\pi^2}{24} \frac{v^2 eH}{\Delta^2} \quad (23)$$

for the superclean limit, and

$$\kappa_{\parallel}/\kappa_0 \simeq 1 + \frac{1}{6\sqrt{3}} \frac{v^2 eH}{\Gamma\Delta} \ln\left(2\sqrt{\frac{\Delta}{\sqrt{3}\Gamma}}\right) \ln\left(\frac{2\Delta}{v\sqrt{eH}}\right) \quad (24)$$

for the clean limit. Finally, off-diagonal thermal conductivity has the simple relation like $\kappa_{\perp} = \kappa_{\parallel}(eB/m)\Gamma_H$ where Γ_H is the scattering rate related to the Hall coefficient.

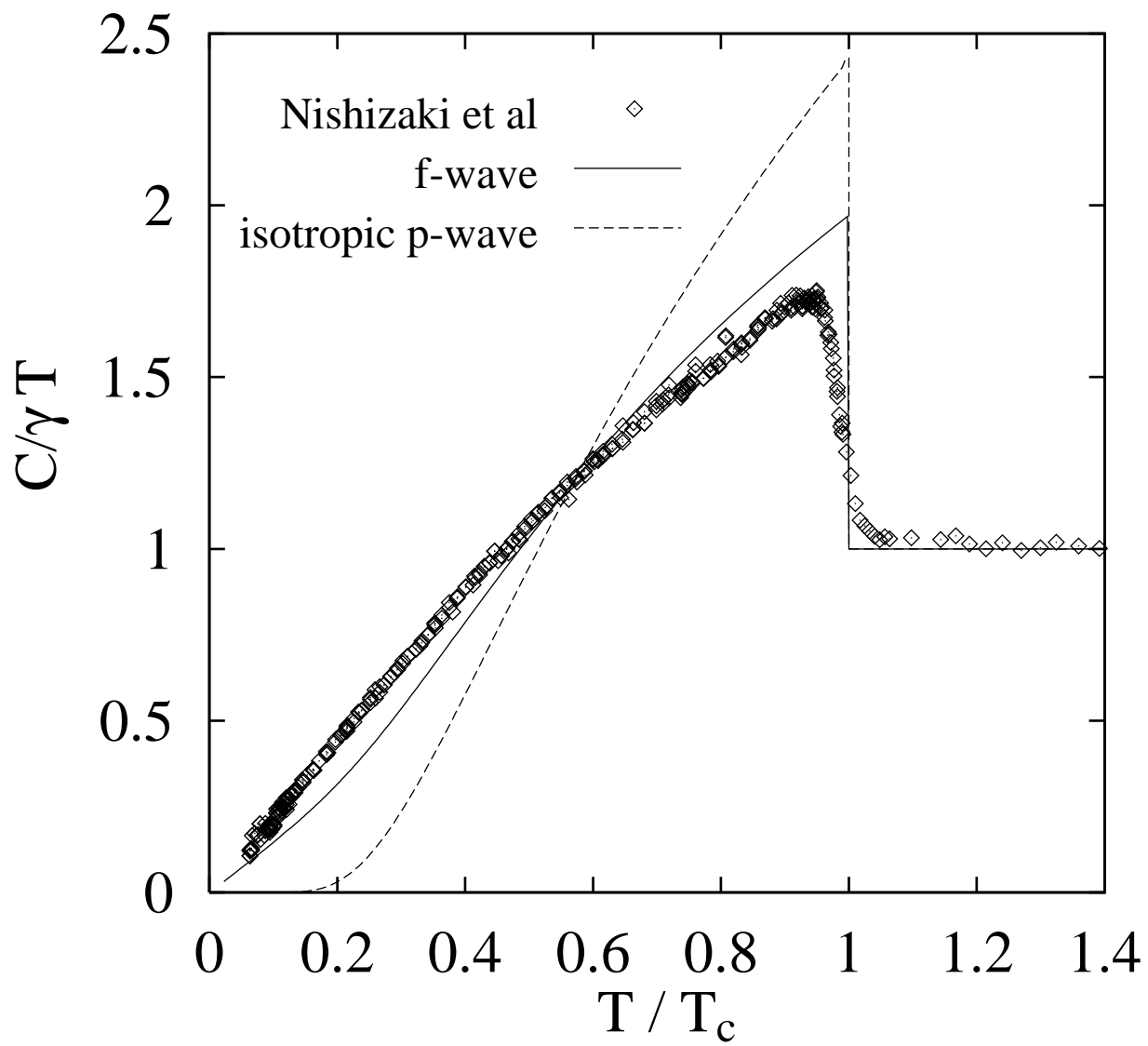
Conclusions. – We have studied theoretically the specific heat and the thermal conductivity tensor in the vortex state of f -wave superconductivity in a planar magnetic field when $H \ll H_{c2}$ and $T \ll T_c$. The quasi-particle relaxation is assumed to be due to the impurity scattering in the unitarity limit.

We find for $H \ll H_{c2}$ and $T \ll T_c$ appreciable $\tilde{\theta}$ -dependence for both the diagonal and the off-diagonal component of the planar thermal conductivity tensor in a planar magnetic field. Although the present $\tilde{\theta}$ -dependences are much smaller than those expected for p -wave superconductors, it is not certain if they are consistent with the thermal conductivity data of Sr_2RuO_4 crystals. Therefore, further works on the thermal conductivity tensor in f -wave superconductors and other unconventional superconductors are highly desirable. On the other hand, the present result should apply for UPt_3 in phase B in a low magnetic field.

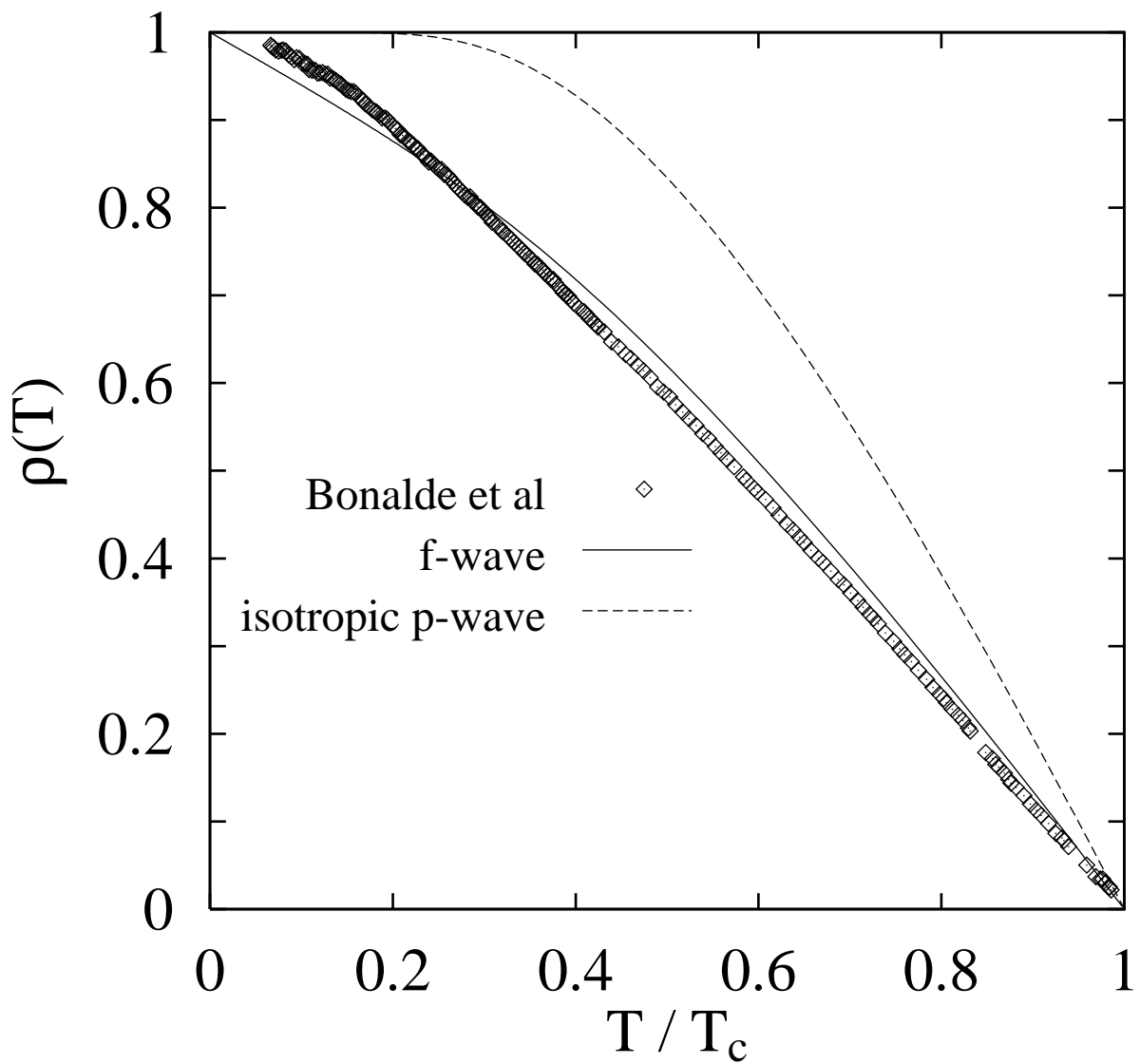
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H. Won and K. Maki, Fig.1



H. Won and K. Maki, Fig.2